Combustion Research Facility News

Volume 22, No. 1 | January/February 2000 | Sandia National Laboratories

CRF Added Space and Research Capability with Phase-II Opening

Sandia National Laboratories' Combustion Research Facility (CRF) celebrated the opening of its Phase-II wing on November 18 with a morning-long symposium on the future of research, a buffet lunch, a ribbon-burning ceremony, and tours of the new facility. The long-awaited Phase-II expansion, which adds over 20,000 ft^2 of laboratory space and 50% more office space to the CRF, includes unique new capabilities in chemistry, imaging, and diagnostics and new facilities for sensor and engine research. Moreover, Phase II offers the external users' community new opportunities for access to the CRF laboratories.

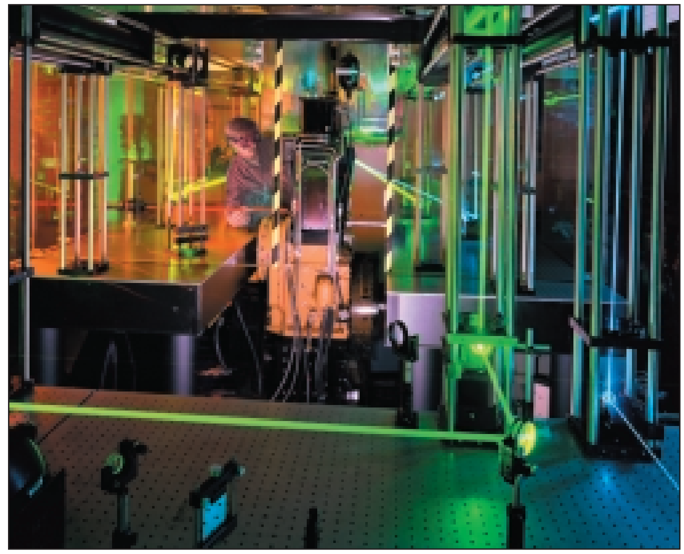
After lunch and the ribbon-burning ceremony, guests toured labs, viewed displays, and heard from the staff about activities underway and planned. Displays and tours focused on the impact of the new facilities on the main areas of CRF activity: Computational Modeling and Simulation, Reacting Flows, Industrial Processes, Combustion Chemistry, Combustion in Engines, and Laser-Based Diagnostics.

Ribbon-burning team (front row from left to right) of Sandia Vice President Dan Hartley, DOE's Director of the Office of Science Martha Krebs (holding the blowtorch that was used to open the CRF in 1981), DOE Chemical Science Division Director Bob Marianelli, and Sandia Executive Vice President Joan Woodard admired their work as the severed Phase-II dedication ribbon hit the ground. Backing up the ribbon-burning team with technical advice were (l-r) Paul Kutler of NASA Ames, Sandia California Vice President Mim John, Stanford Chemistry Professor Richard Zare, Ford Motor Co.'s John McTague (retired), CRF Advisory Board member Pat Flynn of Cummins Engine Company, retired Sandia California Vice President Dick Claassen, and CRF Advisory Board members Dan Seery of United Technologies Research Center and Ron Hanson of Stanford University.

New Diesel Research Engine Became Operational

The engine work at the CRF is devoted to gaining a better understanding of in-cylinder combustion processes with the objective of making engines more efficient and less polluting. Phase II brings the Alternative Fuels Laboratory on line with a new diesel research engine and new diagnostic capabilities. Diesel engines are of particular interest because of their inherently high efficiencies and corresponding promise to reduce greenhouse gas emissions. This laboratory is dedicated to the study of alternative fuels such as alcohols, biodiesel (vegetable-oil-derived esters), ethers, Fischer-Tropsch diesel (paraffins synthesized from natural gas), and even reformulated gasoline. Over the past year, the four-valve, single-cylinder, 1.7-liter base engine, provided by the Caterpillar Corporation, has been modified to provide unparalleled optical access to the combustion chamber.

The successful use of alternative fuels in diesel engines depends on a better understanding of how the chemical and thermodynamic properties of vastly different fuels influence engine efficiency and emissions, particularly mechanisms of soot and NO_x formation. Oxygen-to-carbon ratio, molecular structure, volatility, heat capacity, and density are just a few properties that affect ignition delay, pollutant formation chemistry, fuel-jet penetration, air utilization, and engine "driveability." In addition, understanding glow plug assisted ignition and flame spread in a direct injection diesel engine is critical for operating with low-cetane fuels like alcohols.



The new research diesel engine is readied for use in the Phase-II Alternative Fuels Laboratory. The optical engine has windows in the cylinder wall, piston crown, and piston bowl wall to facilitate the use of a full complement of optical diagnostics, including planar laser-induced fluorescence, laser-induced incandescence, and elastic light scattering. An optical parametric oscillator (OPO) and a dye laser provide tunable light for the spectroscopic measurements. The combustion chamber geometry can be configured to closely match that of the production engine, and users will be able to image soot, NO_x, formaldehyde, and vapor/liquid distributions over the full range of production engine operating conditions.

Experiments at Picosecond Time Scales Will Probe Collisional Processes Important in Laser-Based Combustion Diagnostics

Molecular processes often proceed at collisional rates of 10^9 per second or faster at atmospheric pressure. Direct measurements of such processes, including collisional energy transfer, photoionization, and predissociation, require subnanosecond laser pulses and fast (>1 GHz) detectors. Tunable lasers with 20- to 100-ps pulse durations and transform-limited bandwidths are optimal for studies of collisional processes at atmospheric pressure. For example, picosecond lasers can be used to correct time-resolved laser-induced fluorescence spectra for quenching and to perform degenerate four-wave mixing (DFWM) experiments that are virtually free of interference from slowly formed thermal gratings. The Free Radical Diagnostics Laboratory in the Phase-II wing will offer picosecond lasers along with diagnostic instruments in a configuration that accommodates users.

These facilities will be available to visiting researchers collaborating with the CRF staff in three new areas of scientific investigation: (1) building on the CRF's pioneering work in developing DFWM to see if picosecond lasers improve the sensitivity of DFWM measurements of hydrocarbon flames; (2) improving the accuracy of coherent anti-Stokes Raman spectroscopy (CARS) and laser-induced fluorescence by using picosecond pulses to prepare selected excited states of molecules and observing vibrational and rotational energy transfer; and (3) measuring gas-transport properties of transient species by using gratings generated by laser photolysis.

Symposium Speakers Stimulated and Challenged Guests and Staff

A morning-long symposium entitled "Shaping the Future: The Role of Research in Addressing Critical National Problems," was a highlight of the Phase–II opening celebration. Chaired by DOE's Director of the Office of Science, Martha Krebs, the symposium brought together distinguished speakers Richard Zare, John McTague, Paul Kutler, and George Whitesides.

Professor Zare, Stanford University's Marguerite Lake Wilbur Professor in Natural Science, offered an outsider's view of the Department of Energy and the National Laboratories and pointed out what he considered to be the strengths and weaknesses of the National Labs. According to Professor Zare, the CRF was a good example of the main strength of the National Laboratories, their ability to marshal and integrate diverse talents. McTague, who recently retired as Ford Motor Company's Vice President for Technical Affairs, pointed out to symposium attendees that the globalization of science and technology was now a fact, and that the United States was already reaping the benefits of global leadership. CRF researchers, who have hosted hundreds of foreign post-docs and visitors over the past 20 years, could readily concur. To further make his point, McTague explained that funding of research in the United States by foreign countries had increased tenfold between 1980 and 1995, from $1.5 billion to $15 billion. NASA Ames' Kutler, the Deputy Director for Information Science & Technology, outlined NASA's long-term mission plans, stressing that information technology would be vital to their success.

Professor Richard Zare of Stanford University revealed what he had learned about the National Laboratories as an outsider looking in at DOE research.

Harvard Professor George Whitesides made the point that the assumptions that guided us in the later half of this century may not be true for the next century.

George Whitesides, Mallinckrodt Professor of Chemistry at Harvard University, finished the symposium by reviewing the accomplishments and failures of the last century and proposing that a fruitful way to look into the future might be to examine and challenge current assumptions. He then led the audience through a discussion of four assumptions that he believed were both interesting and widely held. Professor Whitesides concluded that the National Laboratories' future role might be in dealing with complexity of the kind that is found in combinatorial chemistry and stockpile stewardship.

In her remarks, Symposium Chair Martha Krebs reminded the audience that the opening of the second phase of the Combustion Research Facility "was an event deeply worth celebrating." She reminisced about the efforts it had taken to get Phase II built. She also revealed that she had used the CRF as an important model of how to link applied and basic research during her tenure as Director of the Office of Science. She wrapped up the symposium by summarizing the talks and commenting on some of the questions that had come from the audience.

The CRF News is published bimonthly by the Combustion Research Facility, Sandia National Laboratories, Livermore, California, 94551-0969.

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Phase-II Opening Ceremonies Were a Happy Occasion for Everyone Associated with the CRF

Symposium speakers Paul Kutler of NASA Ames and Richard Zare of Stanford University shared ideas about the future of government research with CRF Director Bill McLean and Sandia California VP Mim John.

Joan Woodard, Sandia Executive VP, and Mike Dyer, the Director of the Sandia California Materials and Engineering Sciences Center, leave the Phase-II wing looking like they enjoyed what they saw on their tour of the labs.

Director of the DOE Office of Science and Symposium Chair Martha Krebs reflected on what it had taken to get the second part of the CRF built. She credited Dan Hartley and Bob Marianelli with being instrumental in getting Phase II completed.

CRF's Bob Gallagher answers questions about the Phase-II addition from television news reporter Candice Jones while Stacy Sperber records the interview for Channel 30's 580-680 News.

New and Expanded Labs Focus on Providing Unique Diagnostic Capabilities for the Study of Reactive Flows

The Turbulent Combustion Laboratory, the largest lab in the expanded CRF, provides a complete arsenal of diagnostics to measure reacting flows at Reynolds numbers that are sufficiently high to be consistent with fully turbulent practical combustion devices. Planar laser-induced fluorescence and line Raman measurements are combined in this laboratory to find answers to fundamental questions regarding reaction-zone structure in turbulent flames. This capability allows the CRF to move decisively into research areas where existing data sets and physical understanding are not adequate for rigorous model validation.

The Advanced Imaging Research Laboratory is devoted to developing new imaging diagnostics. The floor space gained in the move to the Phase-II wing makes it possible to better accommodate visiting researchers. Unique capabilities in this lab enable scientists to carry out cold chemistry imaging experiments, reaction rate imaging, and imaging in multiple planes.

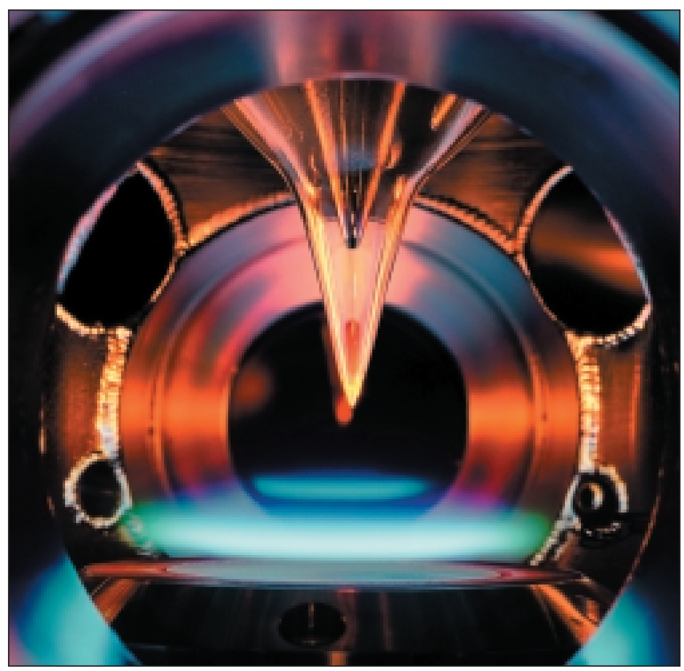
Pioneered at Sandia, the cold chemistry approach makes it possible to study the interplay between turbulent scalar mixing and chemical reactions. Cold chemistry experiments provide a measure of the degree of mixing that cannot otherwise be obtained in a strongly turbulent flow.

Knowledge of local flame burning and heat release rates is required to properly evaluate the performance of combustion systems. A new fluorescence-based reaction-front imaging diagnostic suitable for single-shot experiments is available at the CRF. The measurement is based on taking the pixel-by-pixel product of OH and CH_2O planar laser-induced fluorescence images to yield an image closely related to a reaction rate.

The ability to image native polyatomic flame species like HCO, which fluoresces weakly, is possible with the new capabilities of the Advanced Imaging Research Laboratory. Knowing the concentrations and locations of these polyatomic species permits the investigation of unsteady dynamics found in turbulent flames.

Chemistry Labs Probe Pathways of Combustion Reactions

The combustion process is complex. Given broad domains in fuel chemistry and air/fuel ratios, it is clear that the science and engineering community cannot measure all critical processes needed as input to predictive computer models. Yet the details matter, particularly with respect to pollutant emissions from combustion. Thus, the strategy that has evolved combines detailed characterization of representative processes with development of advanced tools for measurement and computation. In combustion chemistry, we investigate chemical reactivity at varying levels of detail, from time-resolved studies of intramolecular processes to characterization of multireaction environments in idealized combustion devices. In CRF Phase II, three new labs use laser-based methods to investigate the chemical mechanisms of combustion. In two labs, experiments probe the rate and chemical pathways of individual reactions at fixed temperature and pressure. In the third lab, optical and mass-spectrometric detection techniques measure molecular profiles in the multireaction, varying-temperature environment of a low-pressure flame. These experiments, conducted in concert with computational efforts, provide both input to and validation of combustion chemistry models.



The quartz flame probe is the first stage of a new molecular beam sampling instrument designed to measure detailed chemical flame structure. Two mass spectrometers on the molecular beam line detect transient combustion intermediates, and stable reactants and products. The instrument features a vacuum ultraviolet, single-photon photoionization, time-of-flight mass spectrometer and an electron impact, quadrupole mass spectrometer, as well as optical access to the flame.

Sensors Laboratory and Melting Furnace Will Aid Steel and Glass Industries

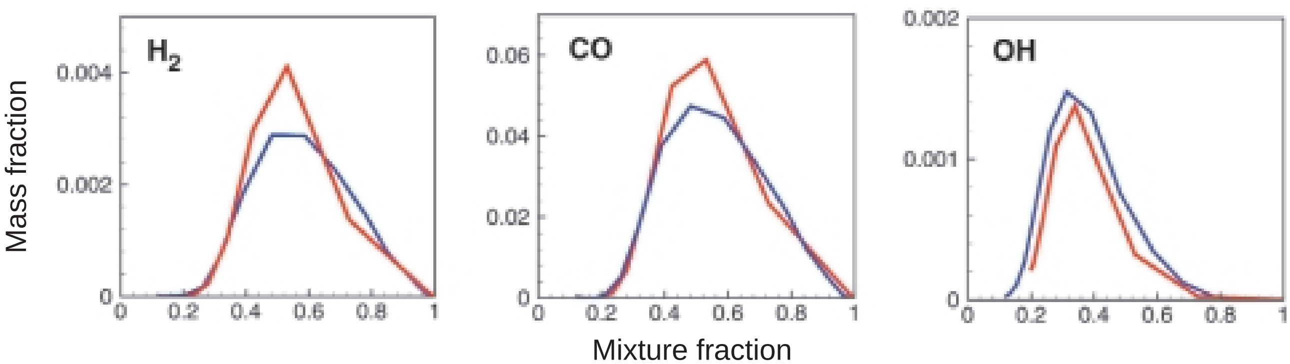
CRF researchers are developing optical sensors to use in the harsh process environments of the glass and steel industries. Both industries are major users of combustion energy and are looking for sensors that afford greater process control and efficiency. The new Phase-II Industrial Sensors Laboratory will focus on the development of such sensors by emphasizing techniques that can produce real-time, in situ measurements of species concentration and temperature in high-temperature, particle-laden environments. One station in the Industrial Sensors Laboratory will include a high-temperature furnace for long-path, particle-free, low-flow experiments.

Research into industrial processes will continue to include a high degree of industrial collaboration. Since 1993, the CRF has been working with the American Iron and Steel Institute to help improve the steelmaking process through better optical diagnostics and process control.

Phase II includes space for the construction of a pilot-scale process furnace that will allow glass manufacturers to study ways to optimize furnace design and melting processes. The furnace, which will be capable of melting seven tons of glass per day, will be outfitted with optical diagnostic equipment that will allow remote measurements of important operational parameters.

Computational Modeling Efforts Benefit from New Laboratory Capabilities

One way to deal with the inherent complexity of combustion is to exploit the potential of computer modeling and simulation. Theorists liken their approach to using computers as molecular microscopes. The Phase-II expansion, while one of expanding experimental capabilities, is directly linked to the computational effort. Models will suggest experiments and experiments will provide the high-quality data necessary to refine and validate models. Current computational approaches include direct numerical simulation and statistical modeling. Direct numerical simulation is accurate and simple, while the statistical method shows promise because it focuses on one dimension and can be run affordably on banks of parallel processors.



Mass fractions generated with the one-dimensional turbulence (ODT) model agree well with experimentally determined mass fractions for CO, OH, and H_2 for the case of a piloted, methane-air jet diffusion flame. The ODT model is a statistical model that captures key mechanisms of multidimensional turbulent flow with a one-dimensional formulation term. Flow is then predicted by a one-dimensional model that evolves according to a random process. Mass fractions of major species were obtained from laboratory measurements of Rayleigh scattering, Raman scattering, and laser-induced fluorescence. Blue lines show the measured values and red lines the values generated by the ODT model.

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